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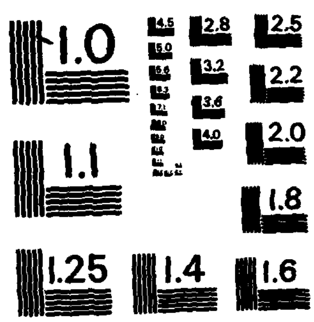

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This report has been reviewed by the Public Affairs Office (PAS) and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nationals.

This technical report has been reviewed and is approved for publication. Publication of this report does not constitute Air Force approval of the report's findings or conclusions. It is published only for the exchange and stimulation of ideas.

Robert J. Peters 11 Jul 85 | Jack Hess

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Based on the classical theory of epitaxial crystal growth, the misfit dislocations and dangling bond densities of abrupt (111) $Hg_{1-x}Cd_xTe$ heterojunctions have been calculated. For the case where $(x_2 - x_1) > 0.1$ the dangling bond density is on the order of $10^{11} cm^{-2}$. Such large dangling bond densities may produce high interface recombination velocities or band-bending at the interface.

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The mercury-cadmium-telluride ($Hg_{1-x}Cd_xTe$) alloy system has become an important semiconductor material for fabrication of infrared detectors. A liquid-phase-epitaxy (LPE) technique is commonly used to grow this semiconductor with the desired Cd content on CdTe substrates. This alloy layer-substrate combination has been referred to as a "lattice matched" system since the lattice constants of HgTe and CdTe differ by only 0.3%. The high performance of p-n junction photovoltaic detectors produced from these epitaxial layers has been taken as evidence of low surface recombination velocities and low defect densities at the $Hg_{1-x}Cd_xTe$/CdTe interface.[1] Consequently, interest has been shown for using LPE techniques to produce more complex double-layer heterojunctions for device applications.[2] These structures are comprised of an n-type layer of composition x_2 on a p-type layer of composition x_1 and, in theory, should have lower leakage currents than p-n homojunction photodiodes. However, the defect structure of $Hg_{1-x}Cd_xTe$ heterojunctions has not been established.

The purpose of this report is to present calculations of the misfit dislocation and dangling bond densities at abrupt $Hg_{1-x_1}Cd_{x_1}Te/Hg_{1-x_2}Cd_{x_2}Te$ heterojunctions where $\Delta x = (x_2 - x_1)$ is a variable. The $Hg_{1-x}Cd_xTe$/CdTe[2] interface is a special case with the variable Δx becoming $(1-x)$. The calculations are made for the (111) plane using the theoretical treatment of Oldham and Milnes.[3] According to this study, the misfit dislocations for (111) heterojunctions may lie in the <011>, <101>, and <110> directions with spacing h between sets as shown in Fig. 1. For pure edge dislocations, h is given by

$$h = \frac{3a_1 a_2^2}{\sqrt{2}\,(a_2^2 - a_1^2)}, \quad a_2 > a_1$$

where a_1 and a_2 are the lattice spacing for x_1 and x_2, respectively, on both sides of the heterojunction. The interface dangling bond density ΔNs is then

$$\Delta Ns = \frac{3}{hc}$$

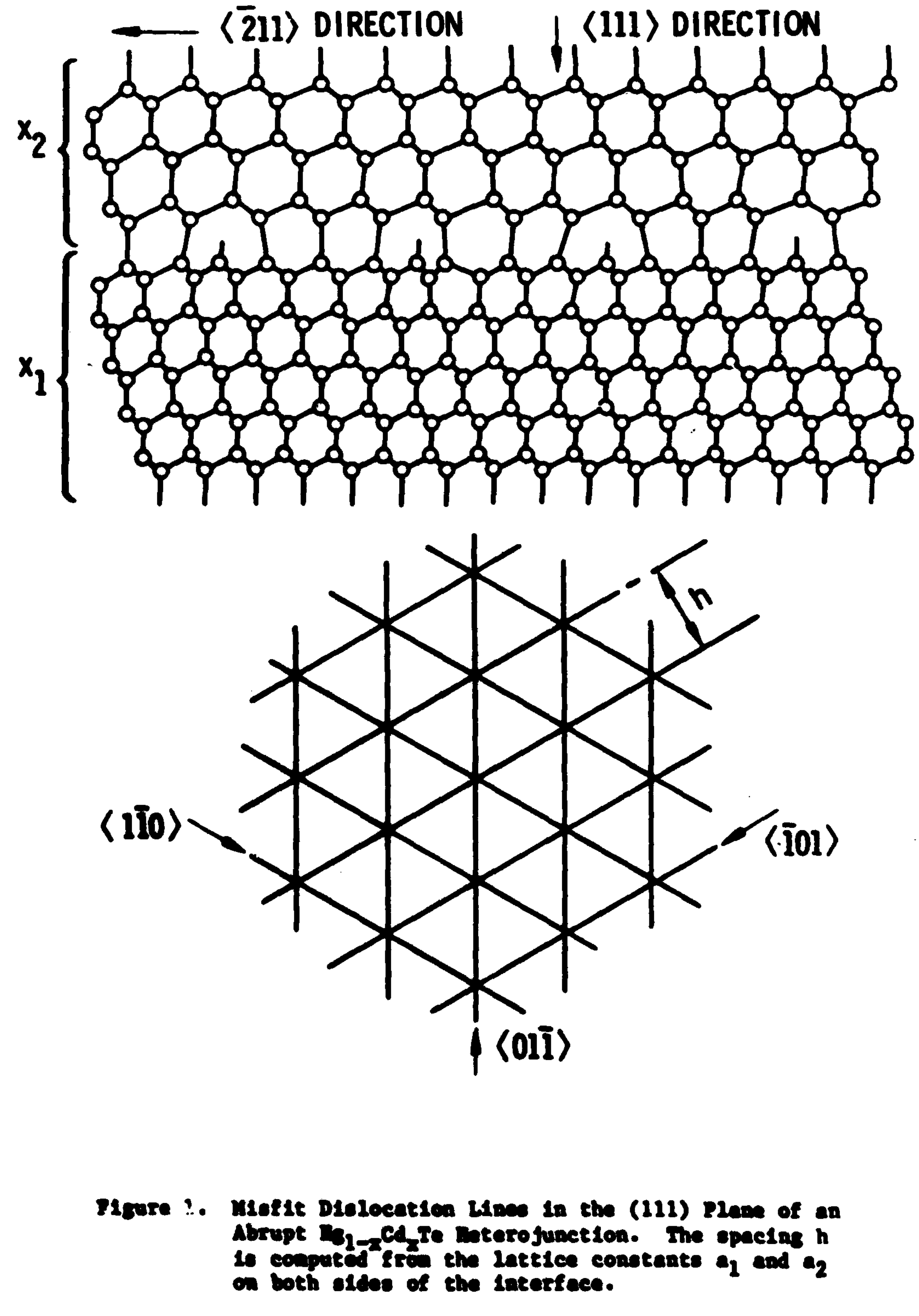

Figure 1. Misfit Dislocation Lines in the (111) Plane of an Abrupt $Hg_{1-x}Cd_xTe$ Heterojunction. The spacing h is computed from the lattice constants a_1 and a_2 on both sides of the interface.

where c is the mean spacing between bonds along the dislocation line and for (111) orientations is given by

$$c = \frac{a_1}{2}\frac{\sqrt{3}}{\sqrt{2}}$$

A recent study of $Hg_{1-x}Cd_xTe$ epitaxial crystal growth[4] has shown that mirror-smooth films can be obtained on $Hg_{1-x}Cd_xTe$ substrates when $\Delta x < 0.03$. Networks of dislocation lines similar to the ones shown in Fig. 1 were observed when $\Delta x > 0.07$.

According to the literature, the lattice constants of CdTe and HgTe at room temperature are 6.4818A and 6.4620A, respectively.[5] The lattice parameter of $Hg_{1-x}Cd_xTe$ varies approximately linearly with x across the entire composition range.[5] The linear thermal expansion coefficients for both materials is $5.0 \times 10^{-6} C^{-1}$ above 300 K.[6,7]

The dislocation line spacing and dangling bond densities for abrupt (111) $Hg_{1-x}Cd_xTe$ heterojunctions are shown in Fig. 2 as a function of Δx. Since the thermal expansion coefficients of CdTe and HgTe are identical, these calculations apply for all LPE growth temperatures.

These dangling bonds should occur in the $Hg_{1-x}Cd_xTe$ epitaxial layer and not in the CdTe substrate since the alloy has the smaller lattice constant. In the case of heterojunctions between two alloy semiconductors, the dangling bonds should occur in the layer with the smaller lattice constant which also has the smaller energy gap. It is well established that such dangling bonds can generate either donor-like or acceptor-like interface states, recombination centers, traps, or in rare instances may remain neutral. The interfacial barrier height generated by donor or acceptor-like states can be estimated from ΔN_s following the method outlined by Many, Goldstein, and Grover[8] for calculating surface potential. According to these calculations, barrier heights in excess of 4 KT/q can be generated whenever $\Delta x > 0.1$.

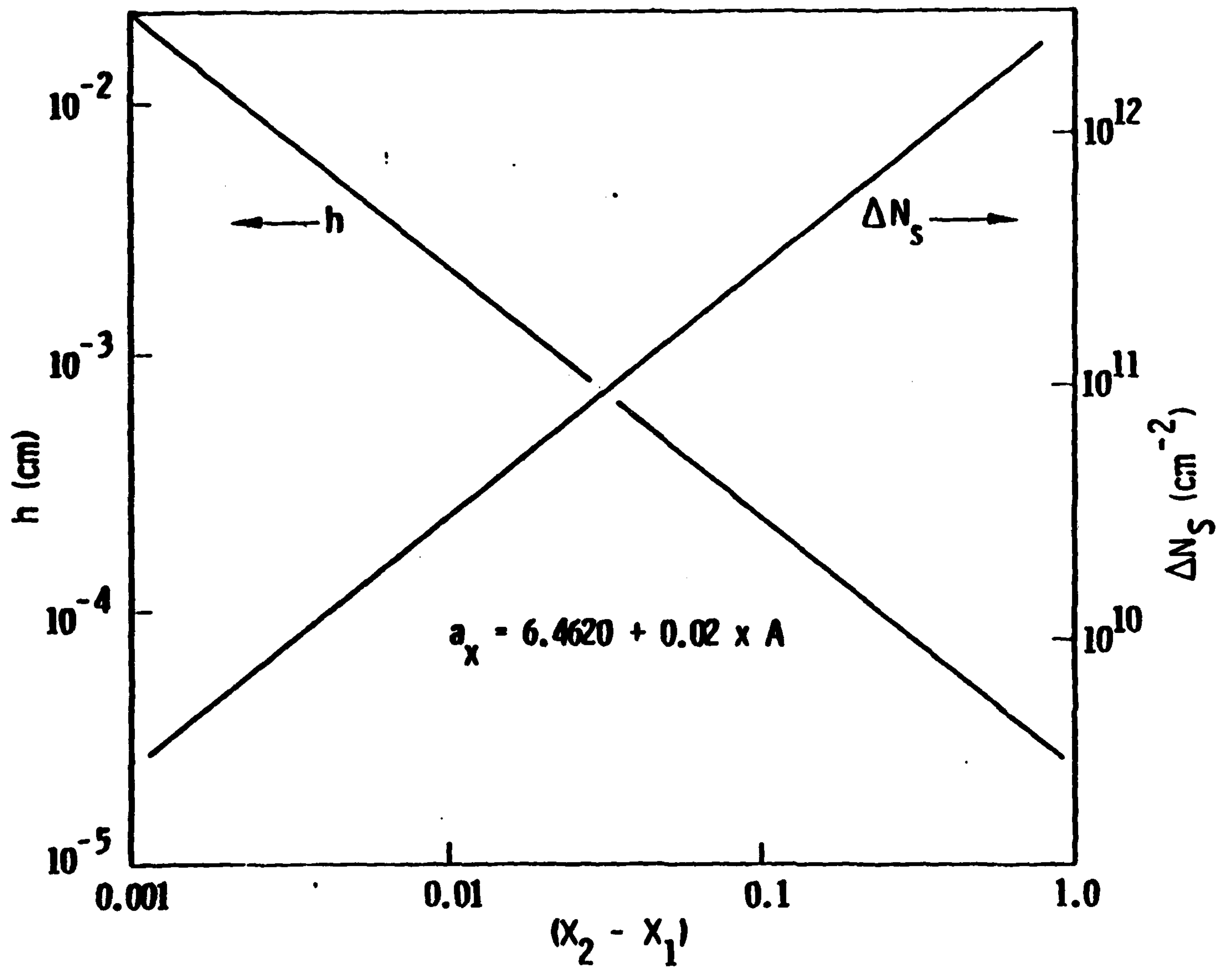

Figure 2. Dislocation Line Spacing h and Dangling Bond Density ΔN_s in Abrupt (111) $Hg_{1-x}Cd_xTe$ Heterojunctions where Compositions on Both Sides of the Interface are x_1 and x_2.

According to this calculation, the $Hg_{1-x}Cd_xTe/CdTe$ interface is far from ideal when $\Delta x > 0.1$. For values of Δx typically encountered in epitaxial growth of detector layers, $\Delta Ns > 10^{12} cm^{-2}$. Such high densities of dangling bonds could easily give rise to high interface state densities and cause severe minority carrier recombination. Of course these interface states may produce band-bending of the proper sign to screen minority carriers from the CdTe interface. This screening could reduce the interface recombination velocity and produce the enhanced "limited volume" diode characteristics reported for p-n junctions fabricated in $Hg_{1-x}Cd_xTe$ epitaxial layers.[1]

In the case of double layer heterojunctions with coincident metallurgical and p-n junctions, the interface states would occur in the depletion region and could produce high recombination rates and excess leakage currents. Any band-bending which would screen thermally generated carriers would also repel optically generated carriers and degrade detector quantum efficiency. Thus, $Hg_{1-x}Cd_xTe$ heterojunctions with $\Delta x > 0.1$ might be expected to exhibit poor photodiode characteristics.

I conclude that abrupt $Hg_{1-x}Cd_xTe$ heterojunction interfaces should have misfit dislocations and dangling bond densities in excess of 10^{11} cm^{-2} whenever $\Delta x > 0.10$. Such large numbers of dangling bonds may cause severe minority carrier recombination and/or band-bending at the interface. Thus, these interfacial defects may play an important role, or may even dominate heterojunction device characteristics.

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